Software

Unintentional fragment handling

Overview

Unintentional fragmentation, also known as transmission-related fragmentation (which can include adducts, dimers, isotopes, and in-source fragmentation), occurs during the mass spectrometry process, where ions may break apart as they pass through the instrument. These additional ion signals complicate data interpretation and reduce reliability unless handled correctly. Thermo Scientific™ Compound Discoverer™ software 3.4 introduces a new feature-based workflow with advanced transmission-related fragment handling capabilities, automating the identification and reduction of transmission-related fragments to enhance data clarity and accuracy.

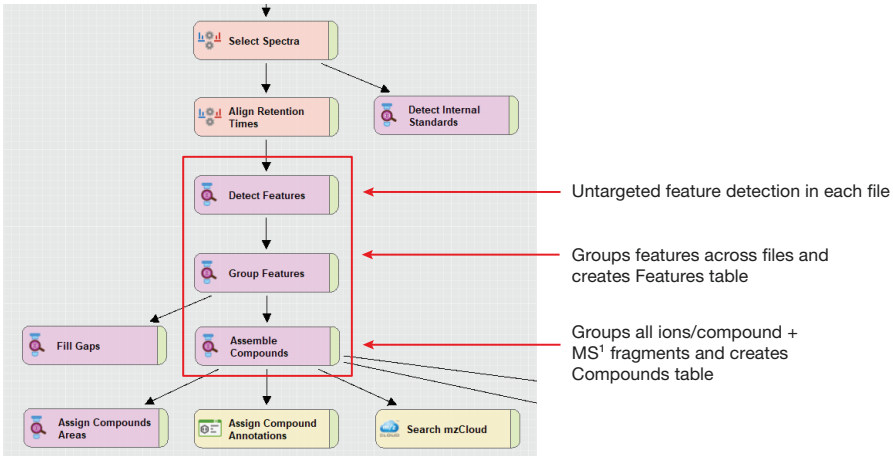
Method

Compound Discoverer software matches transmission-related fragments with the precursor by correlating fragmentation data from the MS^2 scan with peaks that are detected in the full scan. To increase confidence, Compound Discoverer software also makes use of the low collision energy information that is available from the mzCloud™ spectral library. For compounds that can be matched to the data based on authentic standards in mzCloud, Compound Discoverer software automatically retrieves the scan with the lowest collision energy that is available in the spectral library and uses this information to confirm the association between a suspected transmission-related fragment and the precursor.

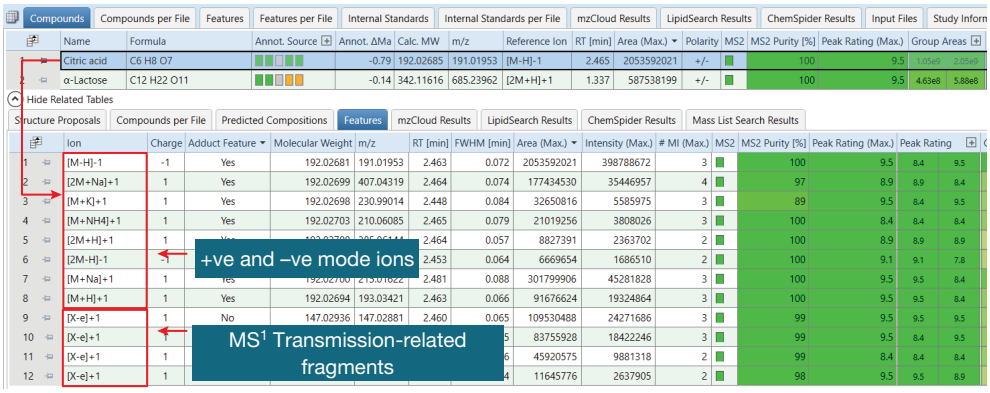
Key features

1. **Automated fragment identification:** The new algorithm in Compound Discoverer software 3.4 automatically identifies transmission-related fragments, which were previously managed manually, and reduces them into a single compound. This feature simplifies your analysis and ensures that data processing is more efficient and less prone to human error.
2. **Comprehensive data reduction:** The automation of transmission-related fragment handling reduces the need for manual intervention, speeding up the data processing workflow so you can focus on data interpretation and analysis.
3. **Enhanced data clarity:** By eliminating chemical noise and artifacts, the software provides a clearer and more accurate representation of the actual compounds present in the sample. This leads to more reliable results in your metabolomics research.
4. **Confident purity assessment:** There is so much stuff in complicated samples, even with best separations and methods you may inevitably have coelutions. The new MS^2 purity column in the compounds table provides a measurable degree of chimerism within an RT window for each compound, helping you build confidence in the clarity of your data.

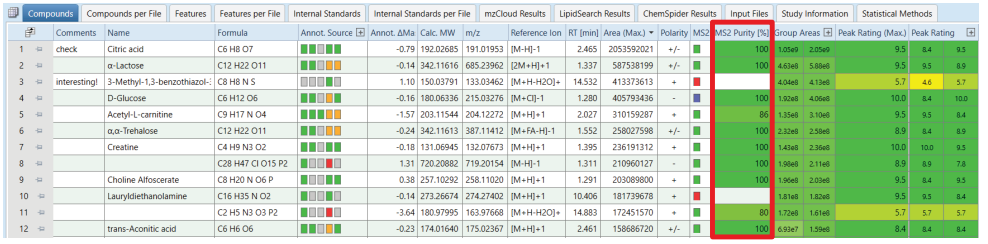
New feature-based workflow



New feature-based workflow | Compounds table with Features sub-table



New columns in the Compounds table



Benefits

- **Efficiency:** Automated processes save time and reduce the workload on researchers.
- **Accuracy:** Improved fragment handling ensures more precise identification of compounds.
- **Data quality:** Reduction of chemical noise and artifacts leads to higher quality data and more reliable results.

Conclusion

The transmission-related fragment handling capabilities in Compound Discoverer software 3.4 streamline the data processing workflow, providing researchers with a powerful tool to achieve more accurate and efficient metabolomics analysis.

Learn more at **thermofisher.com/compounddiscoverer**